

**INTERNATIONAL PRELIMINARY
REPORT ON PATENTABILITY
(SEPARATE SHEET)**

PCT/EP2004/011212

Re Item V

**Reasoned statement with regard to novelty, inventive step or industrial applicability;
citations and explanations supporting such statement**

1. State of the Art

The following documents (D) are referred to in this communication; the numbering will be adhered to in the rest of the procedure:

D1: XP000639763 JACQ P. ET AL.: "PRELIMINARY COMMUNICATION CHIRAL BUTADIENE-TRICARBONYL IRON LIQUID CRYSTAL COMPLEXES: RACEMATES AND ENANTIOMERS"

D2: EP 1 197 791 A (SONY INT EUROP GMBH ;UNIV DURHAM) 17 April 2002
cited in the application

D3: XP000854406 BARMATOV E.B. ET AL.: "INDUCTION OF THE CHOLESTERIC MESOPHASE IN HYDROGEN-BONDED BLENDS OF POLYMERS WITH A LOW MOLECULAR MASS CHIRAL DOPANT"

D4: XP002279441 BARMATOV E. B. ET AL.: "Cholesteric mesophase of the hydrogen-bonded blends of liquid crystalline ionogenic copolymers with a low molecular weight chiral dopant"

D5: XP002279442 TAKEDA M. ET AL.: "Synthesis and properties of trifluoromethylated chiral dopants for ferroelectric liquid crystals"

2. Amendments (Article 34(2)(b) PCT)

The amended claims, filed with the letter of 29.07.2005, do not introduce subject-matter which extends beyond the content of the application as filed, thus meeting the requirements of *Article 34(2)(b) PCT*.

2. Novelty (Article 33(2) PCT) , Inventive Step (Article 33(3) PCT)

The present application meets the criteria of *Article 33(1) PCT*, because the subject-matter of **claims 1-26** is new in the sense of *Article 33(2) PCT* and involves an inventive step in the sense of *Article*

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International application No.

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33(3) PCT.

2.1.

Document **D2**, which is regarded as being the closest prior art to the subject-matter of **claim 1**, discloses (page 4, paragraph 26- page 6, paragraph 41, examples, claims) a liquid crystal mixture for liquid crystal cell comprising a liquid crystal material, which is "BL001" (formally E7)(TM Merck), and a dye, which has a permanent dipole and can be i.a. Morpip (which can form a complex with said LC material, as it is shown in figure 5 of the present application). A liquid crystal cell and the use of the dye in liquid crystal cells (anti-parallel aligned liquid crystal cell, PDLC cell, GH cell) and/or liquid crystal displays is also claimed.

The subject-matter of **claim 1** differs from document **D2** (see page 8, lines 55-58) in that there is 0.5 wt.% of Morpip (or even 1.0 wt.% of Morpip) in the liquid crystal mixture.

The subject-matter of **claim 1** is therefore new (Article 33(2) PCT).

The problem to be solved by the present invention may therefore be regarded as providing an alternative liquid crystal mixture comprising a liquid crystal material and an additive, which can form a complex with said LC material, said LC mixture having improved response times, more specifically turn-on-time and decay-time, improved dielectric anisotropy, increased grey scale response speed of the LC cells and no detrimental loss of LC alignment.

The solution to this problem proposed in claim 1 of the present application is considered as involving an inventive step (Article 33(3) PCT), since it is neither disclosed nor suggested in **D2**, or in any of the documents of the international search report, that the use of 0.01-0.15 wt.% of said additive in such LC mixtures can solve the above problem. Document **D2** does not mention the possibility of using low concentrations of the additive and clearly teaches away from the subject-matter of **claim 1**.

The subject-matter of **claim 1** is therefore inventive (Article 33(3) PCT).

2.2. Other independent claims

The corresponding **independent claims 20, 23 and 25** relate to the use of the composition, a liquid crystal cell and a method of improving the response times, the dielectric anisotropy and the grey scale response speed of an LC cell. The same reasoning applies, *mutatis mutandis*, to the subject-

matter of the corresponding **independent claims 20, 23 and 25**, which therefore is also considered new and inventive.

2.3. Other dependent claims

Claims 2-19, 21-22, 24 and 26 are dependent on claim *1, 20, 23 and 25 respectively* and, as such, also meet the requirements of the PCT with respect to novelty and inventive step.

2.4.

Document **D1** discloses (whole document) mesogenic butadiene-tricarbonyl-iron complexes, which exhibit columnar, cholesteric, smectic A and smectic C* properties. Both smectic mesophases can potentially be used in switchable bistable electro-optic devices and all the mesogenic enantiomers can act as dopants by inducing ferroelectric properties when dissolved in a non-chiral smectic A or C phase. The additive (iron) forms a complex with a liquid crystal compound.

Document **D3** discloses (abstract) the preparation of a family of new hydrogen bonded complexes based on comb-shaped LC copolymers containing alkyloxy-4-oxybenzoic acid mesogenic fragments and chiral dopant molecules, derivatives of pyridine-4-carboxylic acid.

Document **D4** discloses (abstract) the preparation of a family of a new hydrogen-bonded complexes based on comb-shaped LC copolymers containing the monomer units of cyanobiphenyl derivative and n-alkyloxy-4-oxybenzoic acid with a chiral dopant on the base of 4-pyridinecarboxylic acid and L-menthol.

The formation of the complexes of **D1-D4** can implicitly be measured by the methods of **claims 3-6** of the present application. The MOPAC simulations are methods for the study of the chemical behaviour known to the person skilled in the art (see **D5** abstract).

None of the documents **D1 and D3-D5** discloses the use of 0.01-0.15 wt.% of said additive in such LC mixtures, the subject-matter of **claim 1-26** is therefore new and inventive over **D1 and D3-D5**.

10/582399

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S30664PCT

AP3 Rec'd PCT/PTO 12 JUN 2005

Claims

1. A composition comprising a liquid crystal material and an additive, preferably a dopant, wherein said additive is capable of forming a complex with said liquid crystal material, wherein said additive is present in an amount of 0.01-0.15 wt.% of the total composition.
2. The composition according to claim 1, wherein said liquid crystal material and said additive form a complex.
3. The composition according to claim 2, wherein said liquid crystal material and said additive form a complex, as measured by a method selected from the group comprising FTIR, UV-visible absorption, fluorescence, in particular polarized fluorescence, dielectric anisotropy and scanning near-field optical microscopy.
4. The composition according to any of the foregoing claims, wherein said liquid crystal material and said additive form a complex as simulated in MOPAC-simulations.
5. The composition according to claim 4, wherein said MOPAC-simulations comprise the following steps/conditions:
in a computer environment,
 - providing a molecular structure of said liquid crystal material and a molecular structure of said additive,
 - optimizing each molecular structure individually by determining the lowest energy of formation, determining the AM1 and PM3 Hamiltonians and selecting the lowest energy molecular structure that is best fitted by both Hamiltonians,
 - bringing together the optimized individual molecules resulting from the previous step, allowing them to combine, taking into account the charges of atoms, the distribution of charges and the dipole moment of the molecular structures,
 - permutating the previous combination step a number of times, preferably in the range of from 100 – 1000 times, more preferably 200 – 800 times, even more preferably 400 – 600 times and most preferably about 500 times, thus allowing a complex, if any, of said liquid crystal material and additive molecules to form,

- in such complex of molecules, optimizing the structure of the individual molecules so as to determine the lowest energy of formation of the complex and the lowest energy state of the complex.
6. The composition according to claim 5, wherein said MOPAC simulations comprise the additional step:
 - selecting the complex having the lowest energy of formation and calculating from its structure the dipole moment.
 7. A composition comprising a liquid crystal material and an additive, in particular according to any of the foregoing claims, wherein said additive is present in an amount of 0.05 – 0.12 wt.%, more preferably 0.08 – 0.11 wt.% and most preferably around 0.1 wt.% of the total composition.
 8. The composition according to any of the foregoing claims, wherein said additive, when viewed on its own, has no permanent dipole or a dipole ≤ 1 Debye, preferably ≤ 0.1 Debye.
 9. The composition according to claim 8, wherein said additive gains a dipole in the presence of said liquid crystal material and, preferably, upon complex formation with said liquid crystal material.
 10. The composition according to any of claims 7 – 9, wherein said additive is L20 (2,4-dichloro-3,6-diethoxybenzoquinone).
 11. The composition according to any of claims 1 – 7, wherein said additive has a permanent dipole, preferably a dipole ≥ 1 Debye, more preferably ≥ 0.1 Debye.
 12. The composition according to claim 11, wherein said complex formed by said liquid crystal material and said additive has a dipole which is greater than the sum of the individual dipoles of said liquid crystal material and said additive on their own.
 13. The composition according to any of claims 11 – 12, wherein said additive is selected from the group comprising MORPIP (2-{4-[(2,6-dimethylmorpholin-4-yl)(4-methylpiperidin-1-yl)methylene]cyclohexa-2,5-dien-1-ylidene}malononitrile), J6, and

10- γ P3CNQ.

14. The composition according to any of the foregoing claims, wherein said additive is a dye.
15. The composition according to any of the foregoing claims, wherein said liquid crystal material is selected from the group comprising MLC-2038, ZLI-1695, E7 and ZLI-4792.
16. The composition according to any of the foregoing claims, wherein said additive is soluble in said liquid crystal material.
17. The composition according to any of the foregoing claims, wherein said liquid crystal material has a permanent dipole.
18. The composition according to any of claims 1 – 16, wherein said liquid crystal material has an induced dipole.
19. The composition according to any of the foregoing claims, wherein said composition has an order parameter of at least 0.5, preferably of at least 0.7, wherein the order parameter S is defined as:

$$S = \frac{A_{||} - A_{\perp}}{A_{||} + A_{\perp}},$$

wherein $A_{||}$ and A_{\perp} are the measured absorbance values when the director axis of a liquid crystal or liquid crystal mixture is parallel ($A_{||}$) or perpendicular (A_{\perp}) to the propagation axis of an incident polarized light, wherein, more preferably, a parallel state can be achieved by: in the case of a liquid crystal (LC) with positive dielectric anisotropy - inserting a liquid crystal or liquid crystal mixture in a parallel (or antiparallel, or homogeneous) aligned sandwiched cell; and either wherein a perpendicular state can be achieved by either applying an electric or magnetic field to such parallel (or antiparallel, or homogeneous) aligned cell, or alternatively by inserting the liquid crystal or liquid crystal mixture in a homeotropic (or perpendicularly, or vertically) aligned cell; in the case of a LC with negative dielectric anisotropy - inserting a liquid crystal or liquid crystal mixture in a homeotropic (or perpendicularly or vertically) aligned sandwiched cell; and either wherein a parallel state can be achieved by either applying an electric or

magnetic field to such homeotropic aligned cell, or alternatively by inserting the liquid crystal or liquid crystal mixture in a parallel (or antiparallel, or homogeneous) aligned cell.

20. Use of a composition according to any of the foregoing claims in a liquid crystal cell for a liquid crystal display.
21. Use according to claim 20, wherein said liquid crystal cell is a single pixel cell or a multiple pixel cell.
22. Use according to any of claims 20 – 21 for improving the grey scale response time speeds of said liquid crystal cell and/or for shortening the rise and/or decay times of said liquid crystal cell.
23. A liquid crystal cell comprising the composition according to any of claims 1 – 19.
24. Use of a liquid crystal cell according to claim 23 in a liquid crystal display.
25. A method of improving the response time and/or the dielectric anisotropy and/or the grey scale response speed of a liquid crystal, preferably in a liquid crystal cell, comprising the steps:
 - providing a liquid crystal,
 - adding an additive to said liquid crystal, wherein said additive is capable of forming a complex with said liquid crystal, wherein said additive is present in an amount of 0.01-0.15 wt.% of the total composition.
26. The method according to claim 25, wherein said liquid crystal and said additive are as defined in any of claims 1 – 19.

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